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Di-μ-chloro-bis({methyl [*N*,*N*-bis(2-pyridylmethyl)amino]acetate-κ^4N,N',N'',O}copper(II)) bis(perchlorate) monohydrate

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The title compound, $[Cu_2Cl_2(C_{15}H_{17}N_3O_2)_2](ClO_4)_2\cdot H_2O$, contains dichloro-bridged Cu^{II} complexes located on centres of inversion. The solvent water molecule lies on a twofold rotation axis and forms hydrogen bonds to two perchlorate anions.

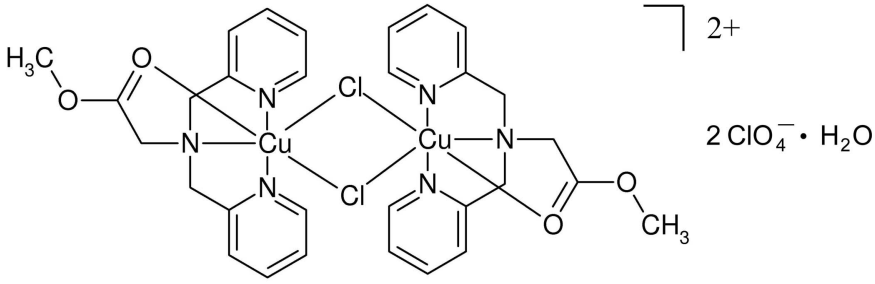
Key indicators

Single-crystal X-ray study
T = 180 K
Mean σ(C–C) = 0.006 Å
R factor = 0.048
wR factor = 0.116
Data-to-parameter ratio = 17.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

In our previous report (Nielsen *et al.*, 2006), we described the dichloro-bridged Cu^{II} complex $[Cu_2Cl_2(bpgH)_2](ClO_4)_2\cdot 4CH_3CN$, where bpgH is the tetradentate bis(2-pyridylmethyl)glycine ligand. The title compound, (I), is closely comparable, but with esterification of the carboxylate groups. Compound (I) contains dichloro-bridged dicopper(II) complexes (Fig. 1), lying on centres of inversion. The coordination geometry around Cu^{II} (Table 1) is closely comparable to that of the bpgH complex (Nielsen *et al.*, 2006), being approximately octahedral with significant elongation of the Cu1—O1 and Cu1—Cl1^{i} bonds [symmetry code: (i) $\frac{1}{2}-x$, $\frac{1}{2}-y$, $-z$] on account of the Jahn–Teller distortion associated with Cu^{II}. The uncoordinated water molecule lies on a twofold rotation axis and forms hydrogen bonds to two perchlorate anions (Table 2).



(I)

Experimental

Esterification of the bpgH ligand to give methyl [bis(2-pyridylmethyl)amino]acetate (bpe) was achieved by a procedure similar to that reported by Rodriguez *et al.* (1997). $Fe(ClO_4)_3\cdot 9H_2O$ (0.1103 g, 0.214 mmol) in 0.5 ml acetonitrile was added to bpgH {bpgH = [bis(2-pyridylmethyl)amino]acetate, 0.1099 g, 0.213 mmol} in 2.5 ml hot acetonitrile. The initial orange precipitate was dissolved by addition of 1 ml water and one drop of 70% $HClO_4$. The solvent volume was reduced by evaporation under gentle heating and a fine orange precipitate of $[Fe(bpe)Cl_3]$ was filtered off (yield 0.021 g). The metathesis reaction (replacing Fe by Cu) was carried out by dissolving the orange solid in a mixture of hot methanol (2.5 ml) and water (0.5 ml), and adding $CuCl_2\cdot 2H_2O$ (0.0078 g, 0.046 mmol) in 0.25 ml methanol. Turquoise crystals were formed after 1–2 d [total yield of

(I) 0.0104 g; *ca* 10% based on bpgH]. IR (KBr, cm^{-1}): ν(C=O) 1612 (*s*).

Crystal data

$[Cu_2Cl_2(C_{15}H_{17}N_3O_2)_2]$-$(ClO_4)_2\cdot H_2O$	V = 3702.9 (2) Å^3
M_r = 957.53	Z = 4
Monoclinic, $C2/c$	D_x = 1.718 Mg m^{-3}
a = 19.1398 (7) Å	Mo $K\alpha$ radiation
b = 8.5993 (3) Å	μ = 1.51 mm^{-1}
c = 24.1605 (8) Å	T = 180 (2) K
β = 111.380 (1)°	Block, turquoise
	0.25 × 0.08 × 0.08 mm

Data collection

Bruker–Nonius X8-APEX-II CCD diffractometer	36620 measured reflections
Thin–slice ω and φ scans	4535 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)	3461 reflections with $I > 2\sigma(I)$
T_{min} = 0.735, T_{max} = 0.889	R_{int} = 0.035
	θ_{max} = 28.3°

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0354P)^2 + 16.3749P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.048	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.116	$\Delta\rho_{max}$ = 1.18 e Å^{-3}
S = 1.11	$\Delta\rho_{min}$ = −0.49 e Å^{-3}
4535 reflections	
254 parameters	
H atoms treated by a mixture of independent and constrained refinement	

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	1.992 (3)	Cu1—O1	2.386 (3)
Cu1—N2	2.068 (3)	Cu1—Cl1	2.2564 (8)
Cu1—N3	1.999 (3)	Cu1—Cl1^{i}	2.9424 (9)
N1—Cu1—N2	83.32 (12)	N3—Cu1—O1	94.26 (10)
N1—Cu1—N3	164.41 (11)	Cl1—Cu1—O1	100.28 (7)
N2—Cu1—N3	81.76 (12)	N1—Cu1—Cl1^{i}	86.91 (8)
N1—Cu1—Cl1	98.23 (8)	N2—Cu1—Cl1^{i}	90.04 (8)
N2—Cu1—Cl1	178.45 (9)	N3—Cu1—Cl1^{i}	88.60 (8)
N3—Cu1—Cl1	96.70 (8)	Cl1—Cu1—Cl1^{i}	90.00 (3)
N1—Cu1—O1	87.51 (11)	O1—Cu1—Cl1^{i}	168.91 (7)
N2—Cu1—O1	79.80 (10)		

Symmetry code: (i) $-x+\frac{1}{2}, -y+\frac{1}{2}, -z$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W···O2A	0.84 (6)	2.18 (2)	2.951 (7)	153 (2)

H atoms bound to C atoms were positioned geometrically and allowed to ride during subsequent refinement, with C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C) for Csp^2, C—H = 0.99 Å and U_{iso}(H) = 1.2U_{eq}(C) for the methylene groups, and C—H = 0.98 Å and U_{iso}(H) = 1.5U_{eq}(C) for the methyl group. The methyl group was also allowed to rotate about its local threefold axis. The O atom of the water molecule is located on a twofold rotation axis at ($\frac{1}{2}, y, \frac{1}{4}$). The unique H atom was placed initially along the O1W···O2A vector then refined with the O1W—H1W distance restrained to be 0.84 (1) Å, the H1W···H1W^{ii} distance restrained to be 1.37 (1) Å [symmetry code: (ii) $1-x, y, \frac{1}{2}-z$], and U_{iso}(H) = 1.5U_{eq}(O). The largest peak in the difference density lies in the vicinity of the perchlorate anion.

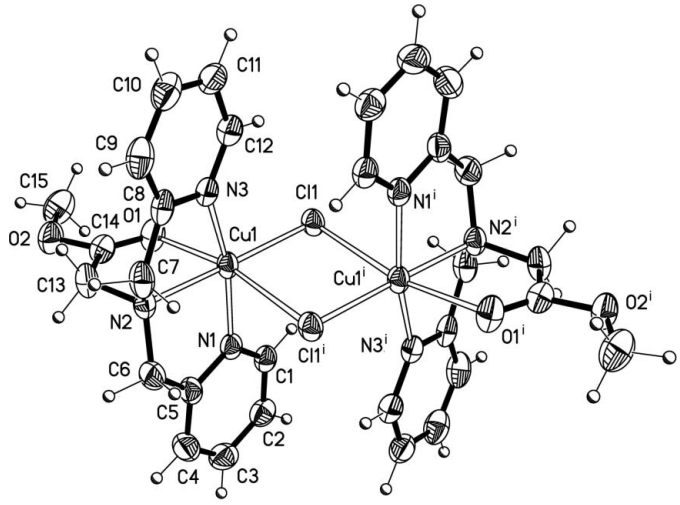


Figure 1
The cationic complex in (I), showing displacement ellipsoids at the 50% probability level for non-H atoms. [Symmetry code: (i) $\frac{1}{2}-x, \frac{1}{2}-y, -z$.]

Data collection: *APEX2* (Bruker–Nonius, 2004); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

We are grateful to the Danish Natural Science Research Council (SNF) and Carlsbergfondet (Denmark) for provision of the X-ray equipment.

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supporting information

Acta Cryst. (2006). E**62**, m2455–m2456 [doi:10.1107/S1600536806034908]

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S1. Comment

In our previous report (Nielsen *et al.*, 2006), we described the dichloro-bridged Cu^{II} complex $[Cu_2Cl_2(bpgH)_2](ClO_4)_2\cdot 4CH_3CN$, where bpgH is the tetradentate bis(2-pyridylmethyl)glycine ligand. The title compound, (I), is closely comparable, but with esterification of the carboxylate groups. Compound (I) contains dichloro-bridged dicopper(II) complexes (Fig. 1), lying on centres of inversion. The coordination geometry around Cu^{II} (Table 1) is closely comparable to that of the bpgH complex (Nielsen *et al.*, 2006), being approximately octahedral with significant elongation of the Cu1—O1 and Cu1—Cl1^{i} bonds [symmetry code: (i) 1/2 − *x*, 1/2 − *y*, −*z*] on account of the Jahn–Teller distortion associated with Cu^{II}. The uncoordinated water molecule lies on a twofold rotation axis and form hydrogen bonds to two perchlorate anions (Table 2).

S2. Experimental

Esterification of the bpgH ligand to give methyl [bis(2-pyridylmethyl)amino]acetate (bpe) was achieved by a procedure similar to that reported by Rodriguez *et al.* (1997). $Fe(ClO_4)_3\cdot 9H_2O$ (0.1103 g, 0.214 mmol) in 0.5 ml acetonitrile was added to bpgH {bpgH = [bis(2-pyridylmethyl)amino]acetate, 0.1099 g, 0.213 mmol} in 2.5 ml hot acetonitrile. The initial orange precipitate was dissolved by addition of 1 ml water and one drop of 70% $HClO_4$. The solvent was reduced by evaporation under gentle heating and a fine orange precipitate of $[Fe(bpe)Cl_3]$ was filtered off (yield 0.021 g). The metathesis reaction (replacing Fe by Cu) was carried out by dissolving the orange solid in a mixture of hot methanol (2.5 ml) and water (0.5 ml), and adding $CuCl_2\cdot 2H_2O$ (0.0078 g, 0.046 mmol) in 0.25 ml me thanol. Turquoise crystals were formed after 1–2 d [total yield of (I) 0.0104 g; *ca* 10% based on bpgH]. IR (KBr, cm^{-1}): ν(C═O) 1612 (*s*).

S3. Refinement

H atoms bound to C atoms were positioned geometrically and allowed to ride during subsequent refinements, with C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C) for Csp^2, C—H = 0.99 Å and U_{iso}(H) = 1.2U_{eq}(C) for the methylene groups, and C—H = 0.98 Å and U_{iso}(H) = 1.5U_{eq}(C) for the methyl group. The methyl group was also allowed to rotate about its local threefold axis. The O atom of the water molecule is located on a twofold rotation axis at (1/2, *y*, 1/4). The unique H atom was placed initially along the O1*W*···O2*A* vector then refined with the O1*W*—H1*W* distance restrained to be 0.84 (1) Å, the H1W···H1W^{ii} distance restrained to be 1.37 (1) Å [symmetry code: (ii) 1 − *x*, *y*, 1/2 − *z*], and U_{iso}(H) = 1.5U_{eq}(O). The largest peak in the difference density lies in the vicinity of the perchlorate anion.

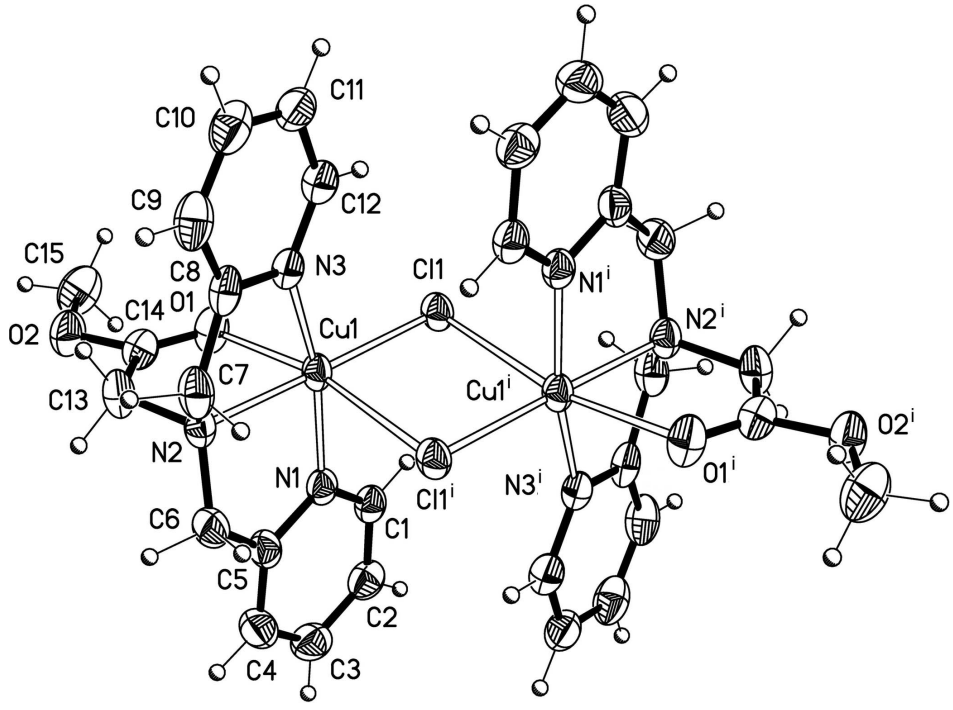

Figure 1

The cationic complex in (I), showing displacement ellipsoids at the 50% probability level for non-H atoms.

Di-μ-chloro-bis({methyl [*N*,*N*-bis(2-pyridylmethyl)amino]acetate- κ^4N,N',N'',O}copper(II)) diperchlorate monohydrate

Crystal data

$[Cu_2Cl_2(C_{15}H_{17}N_3O_2)_2](ClO_4)_2\cdot H_2O$
$M_r = 957.53$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 19.1398\ (7)$ Å
$b = 8.5993\ (3)$ Å
$c = 24.1605\ (8)$ Å
$\beta = 111.380\ (1)°$
$V = 3702.9\ (2)$ Å^3
$Z = 4$
$F(000) = 1952$
$D_x = 1.718$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6163 reflections
$\theta = 2.6–25.4°$
$\mu = 1.51$ mm^{-1}
$T = 180$ K
Block, turquoise
0.25 × 0.08 × 0.08 mm

Data collection

Bruker–Nonius X8-APEX-II CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
thin–slice ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{min} = 0.735$, $T_{max} = 0.889$
36620 measured reflections
4535 independent reflections
3461 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 28.3°$, $\theta_{min} = 3.6°$
$h = -19\rightarrow25$
$k = -11\rightarrow11$
$l = -32\rightarrow26$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.116$
$S = 1.11$
4535 reflections
254 parameters
12 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0354P)^2 + 16.3749P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.18$ e Å^{-3}
$\Delta\rho_{min} = -0.49$ e Å^{-3}

Special details

Experimental. largest difference peak associated with perchlorate anion.

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.34697 (2)	0.21148 (5)	0.052165 (16)	0.02776 (13)
Cl1	0.29214 (5)	0.12462 (10)	−0.04197 (3)	0.0308 (2)
O1	0.47109 (14)	0.1136 (3)	0.07548 (11)	0.0420 (7)
O2	0.57392 (14)	0.0931 (3)	0.15818 (12)	0.0433 (7)
N1	0.38417 (15)	0.4146 (3)	0.03426 (12)	0.0292 (6)
N2	0.39628 (16)	0.2857 (4)	0.13926 (12)	0.0309 (6)
N3	0.31469 (15)	0.0355 (3)	0.09138 (12)	0.0290 (6)
C1	0.38850 (19)	0.4600 (4)	−0.01758 (15)	0.0316 (8)
H1A	0.3715	0.3914	−0.0506	0.038*
C2	0.4168 (2)	0.6031 (5)	−0.02441 (18)	0.0381 (9)
H2A	0.4184	0.6333	−0.0618	0.046*
C3	0.4429 (2)	0.7015 (5)	0.02385 (19)	0.0438 (9)
H3A	0.4628	0.8005	0.0201	0.053*
C4	0.4400 (2)	0.6554 (5)	0.07759 (18)	0.0428 (9)
H4A	0.4584	0.7212	0.1114	0.051*
C5	0.40974 (19)	0.5116 (4)	0.08128 (15)	0.0327 (8)
C6	0.3991 (2)	0.4574 (4)	0.13694 (16)	0.0387 (9)
H6A	0.4411	0.4960	0.1721	0.046*
H6B	0.3519	0.5012	0.1382	0.046*
C7	0.3450 (2)	0.2282 (5)	0.16864 (15)	0.0376 (9)
H7A	0.3714	0.2287	0.2123	0.045*
H7B	0.3008	0.2974	0.1587	0.045*
C8	0.32043 (19)	0.0675 (5)	0.14789 (15)	0.0334 (8)

C9	0.3003 (2)	−0.0413 (5)	0.18131 (16)	0.0431 (10)
H9A	0.3052	−0.0182	0.2210	0.052*
C10	0.2731 (2)	−0.1834 (5)	0.15684 (18)	0.0464 (10)
H10A	0.2583	−0.2584	0.1793	0.056*
C11	0.2675 (2)	−0.2164 (5)	0.09936 (17)	0.0406 (9)
H11A	0.2490	−0.3141	0.0817	0.049*
C12	0.2894 (2)	−0.1040 (4)	0.06837 (16)	0.0359 (8)
H12A	0.2864	−0.1266	0.0291	0.043*
C13	0.4717 (2)	0.2143 (5)	0.16873 (16)	0.0393 (9)
H13A	0.4683	0.1361	0.1977	0.047*
H13B	0.5069	0.2963	0.1913	0.047*
C14	0.5041 (2)	0.1374 (5)	0.12790 (16)	0.0359 (8)
C15	0.6128 (2)	0.0103 (6)	0.1241 (2)	0.0530 (11)
H15A	0.6642	−0.0146	0.1505	0.079*
H15B	0.6143	0.0767	0.0916	0.079*
H15C	0.5859	−0.0860	0.1078	0.079*
Cl2	0.63019 (5)	0.56644 (12)	0.20820 (4)	0.0400 (2)
O2A	0.5727 (2)	0.6096 (8)	0.22630 (19)	0.140 (3)
O2B	0.6611 (4)	0.6883 (6)	0.1886 (3)	0.161 (3)
O2C	0.6033 (2)	0.4633 (7)	0.1608 (2)	0.131 (2)
O2D	0.69066 (19)	0.5047 (5)	0.25644 (14)	0.0698 (10)
O1W	0.5000	0.8911 (6)	0.2500	0.104 (2)
H1W	0.529 (3)	0.834 (2)	0.240 (4)	0.156*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0285 (2)	0.0337 (2)	0.01847 (19)	0.00244 (18)	0.00544 (15)	−0.00104 (17)
Cl1	0.0329 (4)	0.0368 (5)	0.0213 (4)	0.0014 (4)	0.0081 (3)	−0.0041 (3)
O1	0.0367 (14)	0.0550 (18)	0.0315 (14)	0.0112 (13)	0.0092 (11)	0.0021 (12)
O2	0.0302 (14)	0.0528 (17)	0.0411 (14)	0.0081 (13)	0.0060 (11)	0.0030 (13)
N1	0.0231 (14)	0.0333 (16)	0.0286 (14)	0.0048 (12)	0.0062 (11)	−0.0003 (12)
N2	0.0285 (14)	0.0387 (17)	0.0222 (13)	0.0056 (13)	0.0051 (11)	−0.0035 (13)
N3	0.0264 (14)	0.0350 (17)	0.0239 (13)	0.0068 (12)	0.0071 (11)	0.0018 (12)
C1	0.0274 (17)	0.037 (2)	0.0287 (17)	0.0063 (15)	0.0083 (14)	0.0003 (15)
C2	0.0318 (19)	0.040 (2)	0.043 (2)	0.0037 (17)	0.0138 (16)	0.0088 (17)
C3	0.035 (2)	0.035 (2)	0.058 (3)	−0.0010 (17)	0.0135 (18)	0.0038 (19)
C4	0.035 (2)	0.042 (2)	0.045 (2)	−0.0006 (18)	0.0076 (17)	−0.0094 (18)
C5	0.0245 (17)	0.037 (2)	0.0320 (18)	0.0035 (15)	0.0041 (14)	−0.0048 (15)
C6	0.044 (2)	0.039 (2)	0.0285 (18)	0.0042 (17)	0.0076 (16)	−0.0088 (16)
C7	0.0352 (19)	0.057 (2)	0.0205 (15)	0.0055 (18)	0.0098 (14)	−0.0040 (16)
C8	0.0246 (17)	0.051 (2)	0.0238 (16)	0.0111 (16)	0.0076 (13)	0.0045 (16)
C9	0.033 (2)	0.067 (3)	0.0295 (18)	0.0053 (19)	0.0122 (16)	0.0088 (19)
C10	0.036 (2)	0.059 (3)	0.043 (2)	0.003 (2)	0.0125 (18)	0.019 (2)
C11	0.036 (2)	0.039 (2)	0.042 (2)	0.0029 (17)	0.0087 (17)	0.0097 (18)
C12	0.0323 (19)	0.040 (2)	0.0331 (18)	0.0062 (16)	0.0091 (15)	0.0032 (16)
C13	0.0302 (18)	0.055 (2)	0.0268 (17)	0.0025 (18)	0.0038 (14)	−0.0028 (17)
C14	0.0321 (19)	0.039 (2)	0.036 (2)	0.0049 (16)	0.0112 (16)	0.0047 (17)

C15	0.042 (2)	0.064 (3)	0.057 (3)	0.014 (2)	0.023 (2)	0.013 (2)
Cl2	0.0399 (5)	0.0457 (5)	0.0325 (4)	−0.0025 (4)	0.0111 (4)	−0.0039 (4)
O2A	0.057 (2)	0.277 (8)	0.077 (3)	0.049 (4)	0.014 (2)	−0.065 (4)
O2B	0.188 (6)	0.101 (4)	0.199 (7)	−0.001 (4)	0.076 (5)	0.094 (4)
O2C	0.077 (3)	0.189 (6)	0.113 (4)	−0.003 (3)	0.017 (3)	−0.109 (4)
O2D	0.068 (2)	0.092 (3)	0.0477 (18)	0.025 (2)	0.0186 (16)	0.0203 (18)
O1W	0.071 (4)	0.053 (3)	0.201 (8)	0.000	0.065 (5)	0.000

Geometric parameters (Å, º)

Cu1—N1	1.992 (3)	C6—H6A	0.990
Cu1—N2	2.068 (3)	C6—H6B	0.990
Cu1—N3	1.999 (3)	C7—C8	1.487 (6)
Cu1—O1	2.386 (3)	C7—H7A	0.990
Cu1—Cl1	2.2564 (8)	C7—H7B	0.990
Cu1—Cl1^{i}	2.9424 (9)	C8—C9	1.380 (5)
O1—C14	1.209 (4)	C9—C10	1.374 (6)
O2—C14	1.325 (4)	C9—H9A	0.950
O2—C15	1.478 (5)	C10—C11	1.383 (6)
N1—C1	1.343 (4)	C10—H10A	0.950
N1—C5	1.350 (4)	C11—C12	1.378 (5)
N2—C6	1.479 (5)	C11—H11A	0.950
N2—C7	1.489 (5)	C12—H12A	0.950
N2—C13	1.490 (4)	C13—C14	1.496 (5)
N3—C12	1.337 (5)	C13—H13A	0.990
N3—C8	1.357 (4)	C13—H13B	0.990
C1—C2	1.378 (5)	C15—H15A	0.980
C1—H1A	0.950	C15—H15B	0.980
C2—C3	1.379 (6)	C15—H15C	0.980
C2—H2A	0.950	Cl2—O2B	1.370 (4)
C3—C4	1.379 (6)	Cl2—O2A	1.375 (4)
C3—H3A	0.950	Cl2—O2C	1.390 (4)
C4—C5	1.382 (6)	Cl2—O2D	1.413 (3)
C4—H4A	0.950	O1W—H1W	0.84 (6)
C5—C6	1.506 (5)		
N1—Cu1—N2	83.32 (12)	C5—C6—H6A	109.4
N1—Cu1—N3	164.41 (11)	N2—C6—H6B	109.4
N2—Cu1—N3	81.76 (12)	C5—C6—H6B	109.4
N1—Cu1—Cl1	98.23 (8)	H6A—C6—H6B	108.0
N2—Cu1—Cl1	178.45 (9)	C8—C7—N2	109.3 (3)
N3—Cu1—Cl1	96.70 (8)	C8—C7—H7A	109.8
N1—Cu1—O1	87.51 (11)	N2—C7—H7A	109.8
N2—Cu1—O1	79.80 (10)	C8—C7—H7B	109.8
N3—Cu1—O1	94.26 (10)	N2—C7—H7B	109.8
Cl1—Cu1—O1	100.28 (7)	H7A—C7—H7B	108.3
N1—Cu1—Cl1^{i}	86.91 (8)	N3—C8—C9	120.9 (4)
N2—Cu1—Cl1^{i}	90.04 (8)	N3—C8—C7	115.3 (3)

N3—Cu1—Cl1^{i}	88.60 (8)	C9—C8—C7	123.7 (3)
Cl1—Cu1—Cl1^{i}	90.00 (3)	C10—C9—C8	119.6 (4)
O1—Cu1—Cl1^{i}	168.91 (7)	C10—C9—H9A	120.2
C14—O1—Cu1	106.4 (2)	C8—C9—H9A	120.2
C14—O2—C15	116.3 (3)	C9—C10—C11	119.6 (4)
C1—N1—C5	118.6 (3)	C9—C10—H10A	120.2
C1—N1—Cu1	127.3 (2)	C11—C10—H10A	120.2
C5—N1—Cu1	114.1 (2)	C12—C11—C10	118.3 (4)
C6—N2—C7	112.9 (3)	C12—C11—H11A	120.9
C6—N2—C13	112.8 (3)	C10—C11—H11A	120.9
C7—N2—C13	109.1 (3)	N3—C12—C11	122.6 (3)
C6—N2—Cu1	106.2 (2)	N3—C12—H12A	118.7
C7—N2—Cu1	104.3 (2)	C11—C12—H12A	118.7
C13—N2—Cu1	111.2 (2)	N2—C13—C14	115.4 (3)
C12—N3—C8	119.0 (3)	N2—C13—H13A	108.4
C12—N3—Cu1	127.6 (2)	C14—C13—H13A	108.4
C8—N3—Cu1	113.5 (2)	N2—C13—H13B	108.4
N1—C1—C2	122.2 (3)	C14—C13—H13B	108.4
N1—C1—H1A	118.9	H13A—C13—H13B	107.5
C2—C1—H1A	118.9	O1—C14—O2	124.5 (4)
C1—C2—C3	118.9 (4)	O1—C14—C13	125.6 (3)
C1—C2—H2A	120.5	O2—C14—C13	109.9 (3)
C3—C2—H2A	120.5	O2—C15—H15A	109.5
C4—C3—C2	119.5 (4)	O2—C15—H15B	109.5
C4—C3—H3A	120.2	H15A—C15—H15B	109.5
C2—C3—H3A	120.2	O2—C15—H15C	109.5
C3—C4—C5	118.7 (4)	H15A—C15—H15C	109.5
C3—C4—H4A	120.6	H15B—C15—H15C	109.5
C5—C4—H4A	120.6	O2B—Cl2—O2A	113.5 (4)
N1—C5—C4	122.1 (3)	O2B—Cl2—O2C	106.2 (4)
N1—C5—C6	115.8 (3)	O2A—Cl2—O2C	109.6 (3)
C4—C5—C6	122.1 (3)	O2B—Cl2—O2D	104.2 (3)
N2—C6—C5	111.2 (3)	O2A—Cl2—O2D	110.4 (2)
N2—C6—H6A	109.4	O2C—Cl2—O2D	112.7 (3)

N1—Cu1—O1—C14	90.0 (3)	N1—C1—C2—C3	1.3 (5)
N3—Cu1—O1—C14	−74.5 (3)	C1—C2—C3—C4	−0.2 (6)
N2—Cu1—O1—C14	6.3 (3)	C2—C3—C4—C5	−0.9 (6)
Cl1—Cu1—O1—C14	−172.1 (3)	C1—N1—C5—C4	0.0 (5)
Cl1^{i}—Cu1—O1—C14	30.2 (5)	Cu1—N1—C5—C4	177.8 (3)
N3—Cu1—N1—C1	−176.3 (4)	C1—N1—C5—C6	176.6 (3)
N2—Cu1—N1—C1	166.7 (3)	Cu1—N1—C5—C6	−5.6 (4)
Cl1—Cu1—N1—C1	−13.3 (3)	C3—C4—C5—N1	1.0 (6)
O1—Cu1—N1—C1	86.7 (3)	C3—C4—C5—C6	−175.4 (3)
Cl1^{i}—Cu1—N1—C1	−102.9 (3)	C7—N2—C6—C5	−146.3 (3)
N3—Cu1—N1—C5	6.1 (5)	C13—N2—C6—C5	89.4 (3)
N2—Cu1—N1—C5	−10.8 (2)	Cu1—N2—C6—C5	−32.6 (3)
Cl1—Cu1—N1—C5	169.2 (2)	N1—C5—C6—N2	26.7 (4)

O1—Cu1—N1—C5	−90.8 (2)	C4—C5—C6—N2	−156.7 (3)
Cl1^{i}—Cu1—N1—C5	79.6 (2)	C6—N2—C7—C8	156.6 (3)
N1—Cu1—N2—C6	23.9 (2)	C13—N2—C7—C8	−77.2 (3)
N3—Cu1—N2—C6	−151.5 (2)	Cu1—N2—C7—C8	41.7 (3)
O1—Cu1—N2—C6	112.6 (2)	C12—N3—C8—C9	−0.3 (5)
Cl1^{i}—Cu1—N2—C6	−62.9 (2)	Cu1—N3—C8—C9	179.9 (3)
N1—Cu1—N2—C7	143.4 (2)	C12—N3—C8—C7	−176.8 (3)
N3—Cu1—N2—C7	−32.1 (2)	Cu1—N3—C8—C7	3.4 (4)
O1—Cu1—N2—C7	−127.9 (2)	N2—C7—C8—N3	−31.5 (4)
Cl1^{i}—Cu1—N2—C7	56.5 (2)	N2—C7—C8—C9	152.1 (3)
N1—Cu1—N2—C13	−99.1 (3)	N3—C8—C9—C10	−0.9 (5)
N3—Cu1—N2—C13	85.4 (3)	C7—C8—C9—C10	175.3 (3)
O1—Cu1—N2—C13	−10.4 (2)	C8—C9—C10—C11	1.1 (6)
Cl1^{i}—Cu1—N2—C13	174.0 (2)	C9—C10—C11—C12	−0.2 (6)
N1—Cu1—N3—C12	−179.8 (4)	C8—N3—C12—C11	1.2 (5)
N2—Cu1—N3—C12	−162.8 (3)	Cu1—N3—C12—C11	−179.0 (3)
Cl1—Cu1—N3—C12	17.1 (3)	C10—C11—C12—N3	−1.0 (6)
O1—Cu1—N3—C12	−83.8 (3)	C6—N2—C13—C14	−105.3 (4)
Cl1^{i}—Cu1—N3—C12	106.9 (3)	C7—N2—C13—C14	128.4 (4)
N1—Cu1—N3—C8	0.0 (5)	Cu1—N2—C13—C14	13.9 (4)
N2—Cu1—N3—C8	17.0 (2)	Cu1—O1—C14—O2	176.9 (3)
Cl1—Cu1—N3—C8	−163.1 (2)	Cu1—O1—C14—C13	−0.3 (5)
O1—Cu1—N3—C8	96.0 (2)	C15—O2—C14—O1	0.6 (6)
Cl1^{i}—Cu1—N3—C8	−73.3 (2)	C15—O2—C14—C13	178.1 (3)
C5—N1—C1—C2	−1.2 (5)	N2—C13—C14—O1	−9.1 (6)
Cu1—N1—C1—C2	−178.6 (2)	N2—C13—C14—O2	173.5 (3)

Symmetry code: (i) −*x*+1/2, −*y*+1/2, −*z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*···O2*A*	0.84 (6)	2.18 (2)	2.951 (7)	153 (2)